C:\stnweb\Queries\7.str

G1

O

N

N

G2

θ 1

θ 2

31

6

3 4

2 5 1

40

35

34 36

33 38 37

32

θ 1

10 13

9 11 14

8 12 15

7 16

20 23

19 21 24 θ 2

18 22 25

17 26

chain nodes :
    6 31 40
ring nodes :
    1 2 3 4 5 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
    26 32 33 34 35 36 37
chain bonds :
    3-31 4-6 5-40
ring bonds :
    1-2 1-5 2-3 3-4 4-5 7-8 7-12 8-9 9-10 10-11 11-12 11-13 12-16 13-14 14-15
    15-16 17-18 17-22 18-19 19-20 20-21 21-22 21-23 22-26 23-24 24-25 25-26 32-33
    32-37 33-34 34-35 35-36 36-37
exact/norm bonds :
    1-2 1-5 3-31 4-5 4-6 5-40 32-33 32-37 33-34 34-35 35-36 36-37
exact bonds :
    2-3 3-4
normalized bonds :
    7-8 7-12 8-9 9-10 10-11 11-12 11-13 12-16 13-14 14-15 15-16 17-18 17-22
    18-19 19-20 20-21 21-22 21-23 22-26 23-24 24-25 25-26
isolated ring systems :
    containing 1 : 7 : 17 :

G1:Ph,[*1],[*2]

G2:H,Ak

Match level :
    1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom
    12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:Atom
    22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 31:CLASS 32:Atom 33:Atom 34:Atom 35:Atom
    36:Atom 37:Atom 38:CLASS 40:CLASS

```
* * * * * * * * *   Welcome to STN International   * * * * * * * * * *
```

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	Jul 12	BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS
NEWS 4	Jul 30	BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting
NEWS 5	AUG 02	IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields
NEWS 6	AUG 02	CAplus and CA patent records enhanced with European and Japan Patent Office Classifications
NEWS 7	AUG 02	The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available
NEWS 8	AUG 04	Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004
NEWS 9	AUG 27	BIOCOMMERCE: Changes and enhancements to content coverage
NEWS 10	AUG 27	BIOTECHABS/BIOTECHDS: Two new display fields added for legal status data from INPADOC
NEWS 11	SEP 01	INPADOC: New family current-awareness alert (SDI) available
NEWS 12	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS 13	SEP 01	New display format, HITSTR, available in WPIDS/WPINDEX/WPIX
NEWS 14	SEP 14	STN Patent Forum to be held October 13, 2004, in Iselin, NJ
NEWS 15	SEP 27	STANDARDS will no longer be available on STN
NEWS 16	SEP 27	SWETSCAN will no longer be available on STN

NEWS EXPRESS	JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS INTER	General Internet Information
NEWS LOGIN	Welcome Banner and News Items
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
NEWS WWW	CAS World Wide Web Site (general information)

Enter NEWS followed by the item number or name to see news on that
specific topic.

```
  * * * * * * * * * * * * * STN  Columbus  * * * * * * * * * * * * * * * *
```

FILE 'HOME' ENTERED AT 14:19:55 ON 27 SEP 2004

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 14:20:03 ON 27 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

Property values tagged with IC are from the ZIC/VINITI data file

h   eb c   g cg b   cg   eb

provided by InfoChem.

STRUCTURE FILE UPDATES: 26 SEP 2004   HIGHEST RN 752189-88-1
DICTIONARY FILE UPDATES: 26 SEP 2004   HIGHEST RN 752189-88-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

   Please note that search-term pricing does apply when
   conducting SmartSELECT searches.

Crossover limits have been increased.   See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more
information enter HELP PROP at an arrow prompt in the file or refer
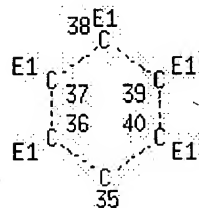to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
L1   STRUCTURE UPLOADED
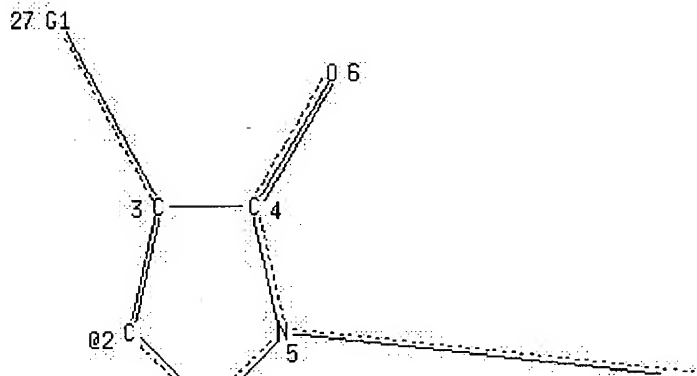
=> d l1
L1 HAS NO ANSWERS
L1   STR

        H 41 Ak 42

Page 1-A

Page 1-B

@30
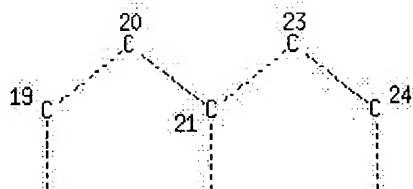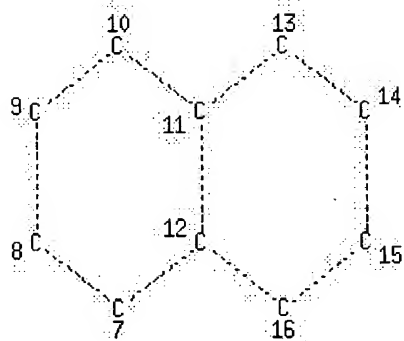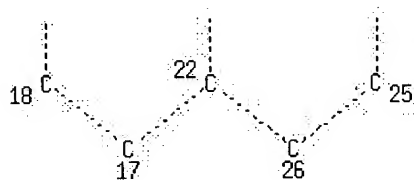
@29
Page 2-A

N
1

G2 34

@31
C

@32
C

C

C

@33
C

C

N
28

Page 2-B

10
C

13
C

9 C

11
C

14
C

8 C

12
C

15
C

7 C

16
C

20
C

23
C

19 C

21
C

24
C

Page 3-B

18 C

22
C

25
C

17
C

26
C
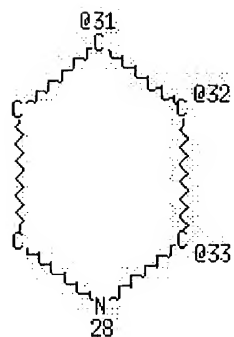
Page 4-B
VAR G1=35/13/24
VAR G2=41/42
VPA 2-29/30/31/32/33 S
NODE ATTRIBUTES:
HCOUNT   IS E1   AT   36
HCOUNT   IS E1   AT   37
HCOUNT   IS E1   AT   38
HCOUNT   IS E1   AT   39
HCOUNT   IS E1   AT   40
NSPEC   IS R   AT   1
NSPEC   IS R   AT   2
NSPEC   IS R   AT   3
NSPEC   IS R   AT   4
NSPEC   IS R   AT   5

h   eb c   g cg b   cg   eb

```
NSPEC    IS C       AT    6
NSPEC    IS R       AT    7
NSPEC    IS R       AT    8
NSPEC    IS R       AT    9
NSPEC    IS R       AT   10
NSPEC    IS R       AT   11
NSPEC    IS R       AT   12
NSPEC    IS R       AT   13
NSPEC    IS R       AT   14
NSPEC    IS R       AT   15
NSPEC    IS R       AT   16
NSPEC    IS R       AT   17
NSPEC    IS R       AT   18
NSPEC    IS R       AT   19
NSPEC    IS R       AT   20
NSPEC    IS R       AT   21
NSPEC    IS R.      AT   22
NSPEC    IS R       AT   23
NSPEC    IS R       AT   24
NSPEC    IS R       AT   25
NSPEC    IS R       AT   26
NSPEC    IS C       AT   27
NSPEC    ·IS R      AT   28
NSPEC    IS R       AT   29
NSPEC    IS R       AT   30
NSPEC    IS R       AT   31
NSPEC    IS R       AT   32
NSPEC    IS·R       AT   33
NSPEC    IS C       AT   34
DEFAULT MLEVEL IS ATOM
MLEVEL   IS CLASS  AT    6 35 36 37 38 39 40 41 42
DEFAULT ECLEVEL IS LIMITED


GRAPH ATTRIBUTES:
RSPEC    1    7  17
NUMBER OF NODES IS   42


STEREO ATTRIBUTES: NONE



=> s 11
SAMPLE SEARCH INITIATED 14:31:29 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     434 TO ITERATE


100.0% PROCESSED     434 ITERATIONS                         0 ANSWERS
SEARCH TIME: 00.00.01


FULL FILE PROJECTIONS:   ONLINE   **COMPLETE**
                         BATCH    **COMPLETE**
PROJECTED ITERATIONS:          7431 TO      9929
PROJECTED ANSWERS:                0 TO         0


L2              0 SEA SSS SAM L1


=> s 11 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 155.00 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 14:31:34 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    9246 TO ITERATE
```

h   eb c   g cg b   cg   eb

```
100.0% PROCESSED     9246 ITERATIONS                            3 ANSWERS
SEARCH TIME: 00.00.01


L3                3 SEA SSS FUL L1


=> file hcaplus
COST IN U.S. DOLLARS                        SINCE FILE        TOTAL
                                              ENTRY          SESSION

FULL ESTIMATED COST                          162.98          163.19


FILE 'HCAPLUS' ENTERED AT 14:31:37 ON 27 SEP 2004
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)
```

```
FILE COVERS 1907 - 27 Sep 2004  VOL 141 ISS 14
FILE LAST UPDATED: 26 Sep 2004  (20040926/ED)


 This file contains CAS Registry Numbers for easy and accurate
 substance identification.


=> s l3
L4                1 L3


=> d l4, ibib abs fhitstr, 1


L4   ANSWER 1 OF 1  HCAPLUS · COPYRIGHT 2004 ACS on STN
```

Full Text

```
ACCESSION NUMBER:          2004:220202  HCAPLUS
DOCUMENT NUMBER:           140:253561
TITLE:                     Preparation of 1,2-dihydropyrazol-3-ones and
                           3-alkoxy-1H-pyrazoles as TNF-α and interleukin
                           lowering agents for the treatment of inflammation
INVENTOR(S):               Dominguez, Celia; Zhang, Dawei; Sham, Kelvin K. C.;
                           Cao, Guo-qiang
PATENT ASSIGNEE(S):        Amgen Inc., USA
SOURCE:                    PCT Int. Appl., 63 pp.
                           CODEN: PIXXD2
DOCUMENT TYPE:             Patent
LANGUAGE:                  English
FAMILY ACC. NUM. COUNT:    1
PATENT INFORMATION:
```

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004022055	A1	20040318	WO 2003-US28067	20030908

```
        W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,
```

```
        CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
        GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
        LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH,
        PL, PT, RO, RU, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA,
        UG, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
    RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG,
        CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC,
        NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ,
        GW, ML, MR, NE, SN, TD, TG
```

hO

R3 OR1   R3   O

R4   N   R4   N-R1
      N   N
      R2   I   R2   II

Cl

III
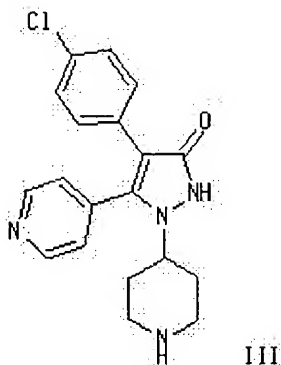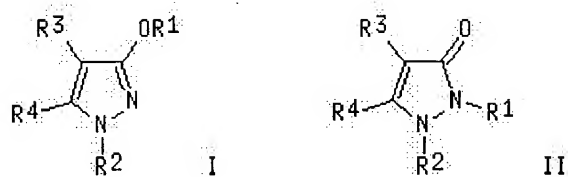
AB   The invention discloses the prepn. of title compds. I and II [wherein R1 =
     H or alkyl; R2 = alkyl, Ph, PhCH2, (alkyl)Rc, (alkyl)Rf, or Rg; R3 and R4
     = independently (un)substituted Ph, naphthyl, or heterocyclyl; Rc =
     independently (un)substituted heterocyclyl; Rf = substituted Rc; Rg =
     substituted alkyl, Ph, or PhCH2; and pharmaceutically acceptable salts
     thereof] as tumor necrosis factor α (TNFα) and interleukin 1,
     6, and 8 (IL-1, IL-6, and IL-8) inhibitors. For example,
     (4-chlorophenyl)acetic acid was condensed with pyridine-4-carbaldehyde in
     acetic anhydride and TEA to give 2-(4-chlorophenyl)-3-(pyridin-4-
     yl)acrylic acid, which was esterified with MeOH in thionyl chloride.
     Cyclization of the acrylate with hydrazine in EtOH, followed by Pd/C
     catalyzed redn., afforded 4-(4-chlorophenyl)-5-(pyridin-4-yl)-1,2-
     dihydropyrazol-3-one. Addn. of 4-oxopiperidine-1-carboxylic acid tert-Bu
     ester in chloroform using sodium triacetoxy boron hydride, hydrogenation
     using Pd/C in EtOH, and deprotection with HCl in ether and dioxane gave
     III. Selected compds. of the invention inhibited lipopolysaccharide-
     activated TNF prodn. in THP1 cells with IC50 values of <20 μM. Also
     disclosed is a method of prophylaxis or treatment of inflammation,
     rheumatoid arthritis, Paget's disease, osteoporosis, multiple myeloma,
     uveitis, acute or chronic myelogenous leukemia, pancreatic β cell
     destruction, osteoarthritis, rheumatoid spondylitis, gouty arthritis,

h   eb c   g cg b   cg   eb

inflammatory bowel disease, adult respiratory distress syndrome (ARDS), psoriasis, Crohn's disease, allergic rhinitis, ulcerative colitis, anaphylaxis, contact dermatitis, asthma, muscle degeneration, cachexia, Reiter's syndrome, type I diabetes, type II diabetes, bone resorption diseases, graft vs. host reaction, Alzheimer's disease, stroke, myocardial infarction, ischemia reperfusion injury, atherosclerosis, brain trauma, multiple sclerosis, cerebral malaria, sepsis, septic shock, toxic shock syndrome, fever, myalgias due to HIV-1, HIV-2, HIV-3, cytomegalovirus (CMV), influenza, adenovirus, the herpes viruses, or herpes zoster infection in a mammal comprising administering an effective amt. of I or II or their pharmaceutical compns. (no data).

IT **671781-23-0P**, 1-(4-Aminocyclohexyl)-4-(naphthalen-2-yl)-5-(pyridin-4-yl)-1,2-dihydropyrazol-3-one

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(TNFα and/or IL inhibitor; prepn. of dihydropyrazolones and alkoxypyrazoles as TNF-α and interleukin lowering agents for treatment of inflammation and related conditions)

RN   671781-23-0 HCAPLUS
CN   3H-Pyrazol-3-one, 1-(4-aminocyclohexyl)-1,2-dihydro-4-(2-naphthalenyl)-5-(4-pyridinyl)- (9CI) (CA INDEX NAME)
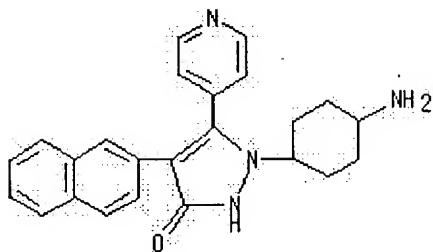
REFERENCE COUNT: 19   THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> file caold

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	7.12	170.31

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-0.70	-0.70

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

h   eb c   g cg b   cg   eb

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

=> d his

    (FILE 'HOME' ENTERED AT 14:19:55 ON 27 SEP 2004)

    FILE 'REGISTRY' ENTERED AT 14:20:03 ON 27 SEP 2004
L1   STRUCTURE UPLOADED
L2   0 S L1
L3   3 S L1 FULL

    FILE 'HCAPLUS' ENTERED AT 14:31:37 ON 27 SEP 2004
L4   1 S L3

    FILE 'CAOLD' ENTERED AT 14:31:47 ON 27 SEP 2004

=> s l3
L5   0 L3

=>

h   eb c   g cg b   cg   eb